Impact of compound-specific mixing and electrostatic interactions on transient transport and solute breakthrough

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Publication date:
2017

Document Version
Peer reviewed version

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ABSTRACT

Compound-specific mixing and Coulombic interactions in advection-dominated flow-through systems have been recently investigated focusing on steady-state transport and lateral mixing (e.g., [1-3]). However, the impact of these effects on transient transport and solute breakthrough has received only limited attention. In this work we present the outcomes of multitracer and multicomponent ionic transport experiments performed in saturated porous media. These bench-scale laboratory experiments were carried out in a quasi 2-D flow-through chamber, in a range of seepage velocity of 0.5-25 m/day. We used pulse injections of multiple tracers (both uncharged and ionic species) through the central inlet ports of the flow-through system. Extensive sampling and measurement of solutes' concentrations at high spatial and temporal resolution (?1500 samples and >3000 measurements) were performed at the outlet of the flow-through setup. The experimental results show that compound-specific effects and charge-induced Coulombic interactions have a remarkable impact on transient transport not only at low but also at high flow velocities. Such effects caused a distinct behavior of measured breakthrough curves of the different solutes also at high Péclet numbers. To interpret the experimental results, we used different modeling approaches: classical advection-dispersion equation (ADE), continuous time random walk (CTRW), dual domain mass transfer equations (DDMT), and a multicomponent ionic dispersion model. The latter is a 2-D transport code [3] based on a multicomponent formulation of the electrostatic coupling between diffusive/dispersive fluxes and allowed us to capture the Coulombic effects during transport of charged species. Furthermore, we considered the flux-related dilution index as a metric of mixing and we determined experimentally its temporal profile for the different solutes measured at the outlet. This metric of mixing, used in connection with the traditional solute breakthrough curves, allowed us to distinguish between plume spreading and mixing, in particular for the cases in which this was not possible based on the sole analysis of integrated concentration breakthrough curves.

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